Handout for advanced CFX course – December 2011

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Note: these workshops are aimed at people who have attended the introduction course for CFX and ICEM and, consequently, basic knowledge of CFX is expected. Some steps will not be explained in full detail anymore. However, new aspects will get more attention in this course.

To use: once a step is finished, click apply or ok – this is always applicable when a different aspect is being discussed

Particle tracking in stirred tank

Purpose: Reminder of introductory course and introduction to particle tracking

Comments: To get a quick solution, we are going to "freeze" the flow field and will only track the particles for a relatively short time. Obviously, more realistic set-ups would take too much time to compute. Also, particle tracking through domain-interfaces can be problematic – there are solutions for this is necessary.

1. Import mesh from results file: 5rps-k-eps-steady2_004.res
2. Create an additional domain for the inner part of the tank and set up the fluid and models (this will be updated for the outer domain as well):
    a. Select part 1244 for this
    b. Select water as the fluid (not air)
    c. Set the domain as rotating at 5 revs/s – axis is global Y
    d. Models:
        i. heat transfer = none
        ii. turbulence = k-epsilon (you can test others, if you have got time)
3. Create boundaries – all of them are walls:
    a. For the outer domain:
        i. Wall
        ii. Baffles
        iii. Shaft
        iv. Surface (can be free slip, but this is not too important in this case)
    b. For the inner domain:
        i. Impeller (rotates with the inner domain)
4. Create interface between inner and outer domain:
    a. Select interfaces for inner and outer domains
    b. Model: frozen rotor
    c. Pitch change: none
5. Try to run it just for a few iterations to see that the set up is correct.
6. Save everything as a backup!

Freezing the flow and particle tracking:

7. Save using another filename.
8. The case could be transient for particle tracking, but this would only make sense here if we switched to transient rotor stator (sliding mesh), which would take a long time to run
9. To create the particles:
    a. Create a new fluid/particle definition in one of the domains
    b. Choose Aluminium (or have a look in the library and pick something else)
    c. Option: Particle transport solid (at the moment there is no difference in the results for the particle transport solid and fluid – extension task: read in help)
    d. Tick particle diameter distribution: and give a specified diameter of 0.5 mm (there are other options – extension task: have a look in the help files)
    e. Switch on buoyancy:
        i. -9.81 m/s^2 in Y direction (0 in X and Z directions)
        ii. Reference density is 997.0 kg/m^3
10. As before: once you apply, the second domain contains the same information
11. Also: there are more tabs in the domain settings
12. Double click outer domain
13. Go to tab Fluid pair models:
    a. Coupling: switch to one-way coupling (fully coupled would mean that the flow is affected by the particles, which is not the case here)
    b. Extension task: read about drag models (in help or online)
14. In Particle Injection Regions... create a new region, then:
    a. Tick particles
    b. Give the cone a centre of 0; 0.2; 0.1
    c. The injection velocity is 0.05 m/s
    d. Look at the options for the cone (extension task: try different settings)
    e. Switch to sphere (instead of cone) and note the different setting options
    f. Specify the number of particles injected: 50 (in transient, one would have to give a number rate, e.g. 30 s^-1, as the particles are injected over time)
    g. OK
15. In solver control go to particle control – tick particle termination control and set maximum tracking time to 1.5 s
16. To “freeze” the flow (can save time in some situations, not only in particle tracking): in menu go to insert/solver/expert parameter
    a. Go to last tab (model over-rides)
    b. Tick solve fluids and solve turbulence and set both values to “f”
17. Write solver file (warnings are okay)
18. Start run in solver with initial file provided
19. After the run is finished:
    a. Look at the particle tracks in post
    b. Compare to streamlines
    c. What are the differences?
20. Extension task: try to run the same case with an injection velocity of 1 m/s

21. Extension task: try to run this in transient mode with sliding mesh (transient rotor/stator in interface for connecting inner and outer domain) – this might take a while
22. Extension task: try to switch on the turbulent dispersion force or the pressure gradient force (in fluid pair models tab in the domain) and have a look in the help files to see what these models do and when they are applicable. Do you see differences? What does this mean?

Multi-phase – example:

1. Start from initial set-up of stirred tank.
2. Create a new material "dispersed drops":
    a. Liquid with density of 1500 kg/m^3
    b. In transport properties: dynamic viscosity is 0.001 kg/m*s
3. In one of the domains: add a second fluid "droplets"
    a. Select the created material
    b. Morphology: dispersed fluid and diameter of 0.250 mm
4. Modelling the multi-phase flow: in one of the domains:
    a. Fluid models tab:
        i. Leave homogenous model unticked (otherwise both phases share the same velocity field)
        ii. Tick homogenous for heat transfer and select none
        iii. Tick homogenous for turbulence and select k-Epsilon
    b. Fluid specific models and fluid pair model: no changes (you can try different drag models, but for such applications this is a separate topic! The help files are a good starting point and there is also more information in literature.)
    c. Initialization: volume fraction
        i. automatic with value: 0.9 for continuous fluid
        ii. automatic with value: 0.1 for droplets
5. Save and write solver file
6. Start from given initial file
7. Note the different tabs/values in solver manager during the run
8. When finished: post-process showing the different volume fractions of the two fluids – for instance on a plane horizontal through the impeller (clearance is 0.072 m)
9. Extension task: read about multi-phase simulations in the help files.
10. Extension task: vary fluid densities - see how this affects the results

Implementing chemical reactions

1. Start with a new case
2. Insert mesh for "pipe with bumps" (in Fluent format)
3. Create boundary conditions:
    a. Inlet: velocity is 0.1785 m/s
    b. Wall=wall
    c. Bumps = wall
    d. Outlet: 0 Pa for relative pressure
4. Solve to check set up and to get an initial file for later
5. In post: have a look at the flow field

6. Go back to the set-up in pre
7. Edit mesh (sometimes very useful):
    a. In tree structure (left side of window) – go into the mesh and un-tick pipe (this way you will not see the pipe's wall anymore and not accidentally select it)
    b. Right click bump1 – edit mesh
    c. Click start picking and select a few elements on bump1
    d. Click in to the field for Move Faces to and rename to cheminlet
    e. Apply
    f. Now the selected elements should be part of the new part "cheminlet"
8. Insert new boundary condition: cheminlet
    a. Inlet with velocity of 0.05 m/s
9. Now we have got the boundaries, but still need the chemical reaction...and for this reacting materials:
    a. In the tree structure: right click water and click duplicate
    b. Rename this copy to reactA
    c. Repeat for reactB and reactC
    d. For most reactions, you would give the program details like density, viscosity and molar mass of the respective reactants and products, but you already know how to change these properties – therefore, we assume that they all behave like water
10. Create a reaction (flame/fire symbol):
    a. Reaction 1 is fine, but you can give it a different name if you want to
    b. It is a single step reaction
    c. In the options, tick reaction or combustion and select Eddy Dissipation in the dropdown menu . This means that the reaction is very fast and only limited by the mixing in the flow, not by the kinetics – extension task: read about the details and other options in the help file.
    d. In the reactants tab: select reactA and reactB as materials and give them stoichiometric factors of 1 and 2, respectively.
    e. In the procucts tab: select reactC and a stoichiometric factor of 3
    f. Therefore: 1A + 2B → 3C (you can give this a lot more complexity – but this allows us to focus on the principle)
11. Now we need a material that combines all of the reactants and "knows" about the reaction
    a. Create a new material and call it reactingmix
    b. Choose the option "reacting material"
    c. Select Reaction 1 in the reactions list
12. Now the simulation needs to use the reaction:
    a. Double click your fluid domain and change the material from water to reactingmix – click apply
    b. In the fluid models tab: there should now be a new option "component models" (otherwise check previous step)
    c. Select reactA and note that the option transport equation is selected
    d. Same for reactB
    e. For reactC: select constraint

f. What does this do? CFX will calculate transport equations for reactA and reactB, while reactC is calculated from the other two values to give unity (extension task: see help for details)

13. Double click inlet
    a. In the boundary details tab: there is a new part “component details”
    b. Set reactA to a mass fraction of 1
    c. reactB should (already) be 0
14. In Cheminlet: reactB should have a mass fraction of 1 and reactA one of 0 (obviously, you can vary this, if you want to)
15. Check if there are any error messages or warnings from CFX. If so, double click them and check what needs to be changed.
16. Save, write the solver definition file and run with the previous as initial values (or without, if you want to try)
17. Once finished, post-process: maybe display the reactant’s mass fractions on a plane? Try a few different things. Do you see any unexpected effects? How could we interpret them?

Periodic boundary (example: rotational periodicity)

1. Start ICEM
2. Create these points: (0/0/0) (0/100/0) (5/0/0) (15/0/0) (0/0/5) (0/0/15) – if you don’t see anything, zoom out/in or rotate the view a bit
3. Reminder: left click=select something; middle click=do something; right click=cancel
4. Create arcs – select from center and 2 points – between the inner (radius=5) and outer (radius=15) points
5. Create lines between the arcs
6. Create a surface from these lines
7. Create another line (axis) between the points (0/0/0) and (0/100/0)
8. Create the rest by driving the curves along the axis – first select axis then the arcs and connecting lines
9. Create surface at the other end as well from the new lines there
10. Create a body between two points
11. Create a block – no need to select anything – just click okay
12. Associate the points – make sure to do this systematically
13. Associate the edges for the arcs to the arcs
14. Change the number of nodes to 10 for the arcs
15. Change the number for the radial nodes to 12 and change the density by selecting from graph in the mesh law dropdown menu - increase the number towards the walls – tick box for copying to parallel edges!
16. Change the axial density to 50
17. Check pre-mesh
18. Create parts for inlet, outlet, innerwall, outerwall, periodic1, periodic2
19. Convert to unstructured mesh
20. Go to output – set solver to Ansys CFX and output the mesh

In CFX Pre:

21. Start with a new case

22. Import the mesh (choose ICEM CFD mesh for the mesh type – mm is fine)
23. Create wall boundaries for innerwall and outerwall
24. Create outlet boundary with 0 pressure
25. Create inlet boundary with 0.0003 m/s inlet velocity
26. Save
27. Double-click default domain and:
    a. Change the fluid to water
    b. Go to fluid models
    c. Set heat transfer to none
    d. Turbulence to laminar (for now)
28. There will be an error message in the lower (right) part of the window – double click it and note that the initial turbulence for the inlet is gone – click okay
29. Now the periodic boundaries:
30. Right-click flow analysis – insert interface
31. Select periodic1 in the first region list and periodic2 in the second one
32. Set Interface models to rotational periodicity and axis to global Y
33. Save, write solver file and run the simulation - should be very fast
34. Have a look at the flow field in post
35. There is very little tangential flow, i.e. flow through the periodic boundaries, and symmetry boundaries would work as well.

Turbulence discussion (continuing with previous example)

36. Now increase the inlet velocity to 0.3 m/s in pre and run again – note that convergence is slower (though still very quick)
37. Run again, but use k-epsilon
38. Do you see any differences in the convergence behaviour or the results?

A different geometry might be more interesting.

39. Let's try the geometry with the bumps:
40. Set the turbulence model to laminar and the inlet velocity to 0.0003 m/s
41. Save, write solver file and run the simulation - this will take a bit more time than before, but still with very good convergence behaviour
42. Now increase the inlet velocity to 0.3 m/s in pre and run again – have a cup of tea, if you want and see if it converges... If it does not finish, stop it.
43. Run again, but use k-epsilon as turbulence model
44. What do you think?